

interaction site and using a computer algorithm to predict a three-dimensional representation of said potential binding agent.

10. The method of claim 1, wherein said plurality of atomic coordinates are as set forth in Table 1.
- 5 11. The method of claim 1, wherein said potential binding agent is designed de novo.
12. A WW domain binding agent identified by the method of claim 1.
13. A method of identifying a WW domain binding agent, said method comprising:
 - 10 (a) defining an interaction site of a WW domain based on a plurality of atomic coordinates of said WW domain;
 - (b) modeling a potential binding agent that fits spatially into said interaction site;
 - (c) determining the ability of said potential binding agent to compete with a WW domain substrate for said interaction site by
15 contacting said potential binding agent with said WW domain in the presence of said WW domain substrate.

09733773-120800

- 5
10
15
20

- 09733773-120800
17. A computer program on a computer readable medium, said computer program comprising instructions to cause a computer to:
- (a) define an interaction site of a WW domain based on a plurality of atomic coordinates of said WW domain; and
- 5 (b) model a potential binding agent that fits spatially into said interaction site.
18. A computer program on a computer readable medium, said computer program comprising instructions to cause a computer to:
- 10 model a potential binding agent that fits spatially into a WW domain interaction site defined by a plurality of atomic coordinates.
19. An isolated crystalline WW domain.
20. The crystalline WW domain of claim 19, wherein said WW domain is a Pin1 WW domain.
21. The crystalline WW domain of claim 20, wherein said Pin1 WW domain has a sequence as set forth in SEQ ID NO:2.
- 15 22. The crystalline WW domain of claim 20, wherein said atomic coordinates of the atoms of said WW domain are as set forth in Table 1.
23. A crystalline complex comprising an isolated WW domain and a WW domain binding agent.
- 20 24. The crystalline complex of claim 23, wherein said WW domain is a Pin1 WW domain.
25. The crystalline complex of claim 24, wherein said Pin1 WW domain has a sequence as set forth in SEQ ID NO:2.
26. The crystalline complex of claim 23, wherein said atomic coordinates of the atoms of said WW domain are as set forth in Table 1.
- 25

27. The crystalline complex of claim 23, wherein said binding agent is a C-terminal domain of RNA polymerase II.
28. The crystalline complex of claim 23, wherein said binding agent has a sequence Tyr-pSer-Pro-Thr-pSer-Pro-Ser (SEQ ID NO:3).